Modal Abundances of Rocks Using Infrared Emission Spectroscopy; K.C. Feely, P.R. Christensen,
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Introduction. Interest in understanding and interpreting emission spectra produced by geologic materials has greatly increased during the last few years due to data return from several spectrometers mapping the Earth and the expected data from Thermal Emission Spectrometer (TES). Theories of vibrational spectroscopy describe how the interaction of electromagnetic energy with molecules produces characteristic peaks in infrared spectra and explain why each mineral can be identified by a unique infrared spectrum [1, 2, and others]. Studies have also determined that infrared spectra of granular mineral mixtures are equivalent to the weighted linear combination of the individual mineral spectra [3, 4]. Since rocks are essentially "mineral mixtures," the objective of this research is to deconvolve the measured infrared emission spectra and calculate the modal abundances of a suite of igneous rocks to determine the accuracy obtainable by this technique. Error is determined by comparing the modes determined spectroscopically with those determined petrographically.

Data Collection. Rock samples used in this work were selected from ASU petrology collections and include compositional suites of granites, rhyolites, and andesite/basalts. All are representative of the basic physical properties of the rock type, have modal abundances determined by traditional petrographic methods, and are available as hand samples with maximum dimension of 5 to 11 cm. An infrared spectrum of each rock sample was collected using the Mattson Cygnus 100 interferometric spectrometer and the basic technique described in Ruff [5]. Spectra of minerals, necessary for deconvolution of the rock spectra (see below), were obtained from the Thermal Emission Spectrometer Mineral Library.

Spectra were deconvolved with a least squares fit algorithm that employs matrix algebra to solve a set of linear equations that represents the rock spectrum as a composite of the mineral spectra [4]. Required input includes the measured rock (mixed) spectrum and a suite of possible mineral endmember spectra. Produced from this are a model of the rock spectra, a list of minerals present with modal percentages, and error of the analysis.

Results and Analyses. Modal analyses resulting from the deconvolution of rock spectra were compared to the modal analyses already determined petrographically, hereafter referred to as the "known modes." At a first level of analysis, the deconvolution algorithm was usually able to identify the minerals composing at least 5% of the rock, with the exception of biotite in the granites and olivine in the basalts. Statistically, all of the primary minerals were identified in 21 out of 26 granite samples, 5 out of 8 rhyolite samples, and 9 out of 11 andesite/basalt samples (respectively 81%, 63%, and 82%.) Figure 1 shows the measured and the best fit model spectra for two representative samples: a fine-grained, olivine-subalkali basalt and a coarse-grained, I-type granite. For both of these examples, all of the known minerals were identified, except olivine in the basalt.

At a second level of analysis, the deconvolution algorithm calculated quantitative modal abundances, comparable to those determined petrographically. Modal analyses of primary minerals composing the granite, rhyolite, and basalt samples were calculated with an average accuracy of ±7% deviation from the known modes (Fig. 1b & 1c). Total feldspar composition was used for basalts which contain feldspars too fine grained to differentiate using traditional methods. Closer examination of feldspar types in granites show two consistent trends: plagioclase was underestimated, while K-feldspar was overestimated (Fig. 1d). Further work will examine whether or not these observed trends can be correlated either to the physical properties of the rock, such as grain size or texture, or to spectral characteristics of the minerals.

Conclusions. Infrared emission spectra collected from large rock samples can be successfully deconvolved to determine the quantitative mineral composition. With noted exceptions, primary minerals in any igneous rock type can be identified within an average of ±7% of the actual modal abundance. This technique can be applied to remotely sensed spectroscopic data from TES, and other instruments, to identify rocks with detailed mineral assemblages.

References. [1] Lyon, R. J. P., NASA Tech. Note D-1871, 1963. [2] McMillian, P.F., and A.M. Hofmeister, Chpt. 4, *Reviews in Mineralogy*, Vol.18, 1988. [3] Thomson, J. L., and J.W. Salisbury, *Rem. Sens. Env.*, Vol. 45, pp. 1-13, 1993. [4] Ramsey, M. S., Ph.D. Dissertation, ASU, 1996. [5] Ruff, S.W., *et. al.*, *JGR*, In press.

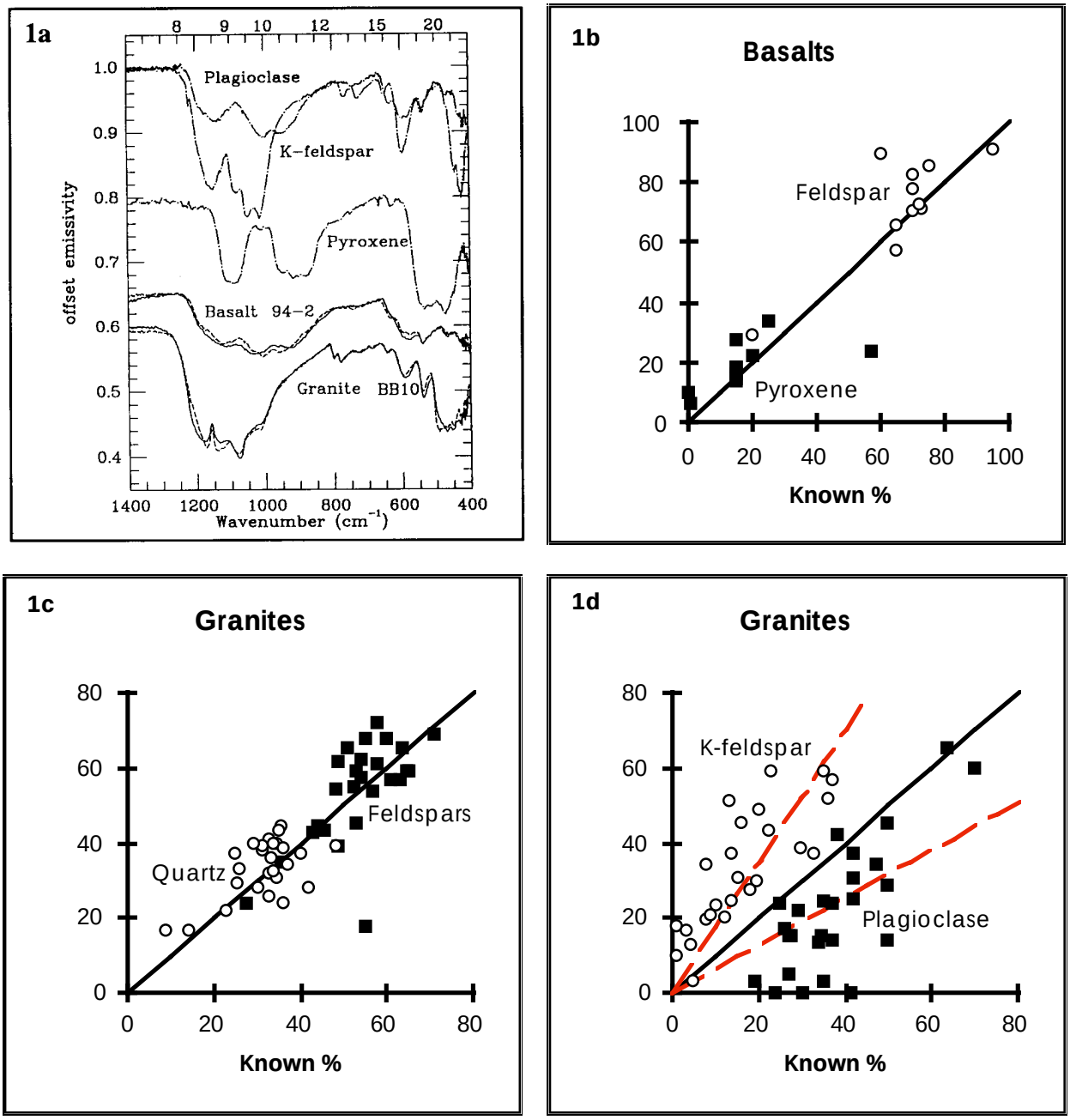

Figure 1: (a) Examples of mineral (top three) and rock spectra (bottom two). Measured rock spectra are shown by a solid line with the associated model shown by a dashed line. (b-d) Quantitative modal analysis results for primary minerals in the granite and basalt suites. Points that fall on the diagonal line are a "perfect match" between spectroscopic and petrographic analyses.